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Disciplines
Engineering | Materials Science and Engineering | Metallurgy

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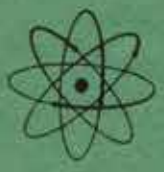

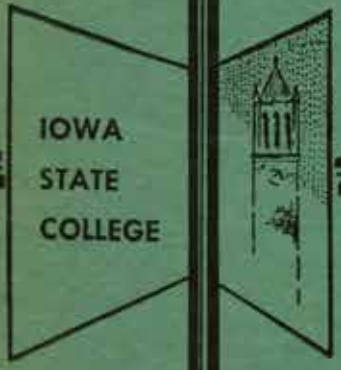

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This report is the fifth and last in a series. The previous reports listed the compounds of elements as follows:

ISC-795, Lithium, Sodium, Potassium, and Rubidium

ISC-812, Beryllium, Magnesium, and Calcium

ISC-906, Copper, Silver, and Gold

ISC-1047, Zinc, Cadmium, and Mercury

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
AlLi	cubic	a=6.37	B32	X-ray powder, thermal and microscopic data	1,2, 3,4
$AlLi_2$				Thermal and micrographic analysis; forms peritectically at 521°C.	3,4
θ"-Al_2Cu	tetragonal	a=4.04 c=7.9		Single crystal x-ray data; first precipitate formed on ageing of Al-Cu alloys.	162, 163
θ'-Al_2Cu	tetragonal	a=4.04 c=5.8	C1	Single crystal x-ray data; this is an intermediate precipitate observed in age-hardened Al-Cu alloys.	9,163
θ-Al_2Cu	tetragonal	a=6.066 c=4.874	C16	X-ray powder data; narrow range of homogeneity of 67.1-68.05 a/o Al at 548°C.	11,13, 163
η_1-AlCu	orthorhombic	a=4.095 b=12.02 c=8.652	$[C_{mmm}]$	X-ray single crystal data, thermal analysis; high temperature phase.	13,16
η_2-AlCu	orthorhombic	a=6.89 b=4.09 c=9.89		X-ray powder data, thermal analysis; low temperature phase.	13,17
δ_1-Al_3Cu_4	hexagonal	a=8.10 c=10.00	$[P6/mmm]$	X-ray single crystal data, thermal analysis; high temperature modification.	13,16, 17
δ_2-Al_9Cu_{12}	probably monoclinic	a=7.07 b=4.08 c=10.02 β=90°38'		X-ray powder data; low temperature modification; A=21.	17
γ_2-Al_2Cu_3	pseudocubic	a=8.69	$\sim D8_{1-3}$	X-ray powder data; exists from 20.7-22.5 w/o Al; the structures Al_4Cu_9, $Al_{19}Cu_{32}$, and Al_2Cu_3 are so closely related that no two-phase regions can be found among them.	17
γ_1-$Al_{19}Cu_{32}$	probably monoclinic		$\sim D8_{1-3}$ probably $[C_s^3-C_m]$	X-ray powder data; stable at 35.3-38.1 a/o Al; A=102; a modification of Al_4Cu_9; has deformed γ-brass structure; parameter for pseudocubic cell of 51 atoms is a= 8.72 Å	12,13, 17

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
γ-Al_4Cu_9	cubic	a=8.7040	~$D8_{1-3}$	X-ray diffraction data with intensity measurements; thermal analysis; exists from 16-18.8 w/o Al.	10, 11, 13,17
β-$AlCu_3$	cubic	a=2.95	A2	X-ray powder data, thermal and microscopic analysis; disordered structure, stable only at higher temperatures; lattice constant measured at 600°C.	5, 10, 11,13, 14,28
β_1-$AlCu_3$	cubic	a=5.82	DO_3	X-ray diffraction data with intensity measurements; thermal and microscopic analysis; ordered structure; on further cooling of alloys < 13.1 w/o Al, β_1 structure transforms to a β' structure which is a distorted γ' structure (Cu_3Al); β' can be converted to γ' by mechanical deformation.	5,10, 13,14
γ'-$AlCu_3$	ortho-rhombic	a=4.52 b=5.21 c=4.23		X-ray powder data, thermal analysis; structure is a distortion of the β_1 phase; also indexed as hexagonal (14) with a 2.60, c 4.106 Å.	13, 14, 36,37
Al_2Ag_3	hexagonal	a=2.871-2.885 c=4.663-4.582	A3	X-ray powder data; range of homogeneity of 27-40 a/o Al; (22) says no intermetallic compound exists here, only a solid solution.	18, 21,22
β-$AlAg_3$	cubic	a=3.25	A2	High temperature x-ray powder data; phase exists above 600°C; random arrangement of atoms on lattice sites.	18, 21
μ-$AlAg_3$	cubic	a=6.934	T^4-- $P2_13$	X-ray diffraction data with intensity measurements; micrographic analysis; low temperature phase; phase is of variable composition; A 20; 15 Ag and 5 Al atoms randomly arranged.	19, 20,21
Al_2Au	cubic	a=6.00	C1	X-ray powder data with intensities.	23,24
AlAu	cubic	a=6.05	B3	X-ray powder data; instead of this structure (23) and (25) report a complex powder pattern.	23, 25,26
$AlAu_2$				Thermal analysis and metallography.	23,25
Al_2Au_5				Thermal analysis and metallography; compound may be Al_3Au_8; structure is probably similar to γ-brass, but apparently is hexagonally distorted.	23

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
$AlAu_4$	cubic	a=6.919-6.923	$[T^4-P2_13]$	X-ray powder data; formerly called $AlAu_3$; undergoes an order-disorder transformation at elevated temperatures to A2 structure with a=3.24 Å at 500°C.	6,23, 25,27
Al_3Mg_2	cubic	a=28.19	$[O_h^7-Fd3m]$	Laue and Weissenberg x-ray data; thermal analysis; complicated structure with 1172 atoms/cell; earlier reported as hexagonal with a=11.40, c=17.91Å (31)	29, 30,31, 34,40
~ Al_9Mg_{11}				X-ray powder data, thermal analysis; exists below 410°C; phase diagram in this region somewhat uncertain.	29, 34,35, 38,40
$Al_{12}Mg_{17}$	cubic	a=10.469-10.591 (51.6-61.5 a/o Mg)	A12	X-ray powder data, thermal analysis.	29,31, 39,40
Al_4Ca	tetragonal	a=4.36 c=11.09	$D1_3$	X-ray powder data; narrow range of homogeneity.	41
Al_2Ca	cubic	a=8.038	C15	"	41,42
Al_4Sr	tetragonal	a=4.46 c=11.07	$D1_3$	Powder and single crystal x-ray data; range of homogeneity at 700°C is ~15-25.7 a/o Sr.	43
AlSr	cubic	a=15.8		Powder and single crystal x-ray data; A=116; the structure is probably a superstructure based on the B2 structure.	43
Al_4Ba	tetragonal	a=4.540 c=11.16	$D1_3$	Laue and rotation x-ray data; thermal analysis.	44
Al_2Ba				X-ray diffraction data, thermal analysis.	45
AlBa	hexagonal	a=6.01 c=17.78		Single crystal x-ray data, thermal analysis; A=16.	45
Al_2Ba_9				Existence reported on basis of thermal analysis; x-ray diffraction data fails to verify existence.	45
$AlBa_9$				"	45

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Al-Zn				No compounds formed.	46
Al_4La	tetragonal	a=4.42 c=10.2	$D1_3$	X-ray powder data, thermal analysis, microscopic examination.	32,48
Al_2La	cubic	a 8.131	C15	"	32,33,48
AlLa				Thermal analysis, microscopic examination.	32,48
Al_2La_3				"	47
Al_4Ce	tetragonal	a=4.374 c=10.12	$D1_3$	X-ray powder data, thermal analysis.	32
Al_2Ce	cubic	a=8.11	C15	"	32,49
AlCe	orthorhombic	a=9.27 b=7.68 c=5.76	probably C_{2v}^{12} -- $Cmc2_1$	X-ray powder data, thermal analysis and metallography; indexing only probable.	32,47, 52,85
α-$AlCe_3$	hexagonal	a=7.043 c 5.451	DO_{19}	X-ray powder data, thermal analysis and metallography; stable below 230°C.	85
β-$AlCe_3$	cubic	a 4.985	L12	X-ray powder data, thermal analysis and metallography; exists above 230°C; these two modifications of Ce_3Al were found by (85), instead of Ce_3Al_2 postulated by (47).	85
Al_4Pr				Thermal analysis, microscopic examination; two allotropic forms exist, transforming at 1018°C.	50,133
Al_2Pr				Thermal analysis, microscopic examination.	50
AlPr				"	50
Al_2Pr_3				"	47
AlNd	cubic	a=3.74	B2	X-ray diffraction data.	51

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Al_4Pu	orthorhombic	a=4.42 b=6.26 c=13.66	$[D_{2h}^{28}$-- Imma]	Powder and single crystal x-ray data.	53,55
Al_3Pu	hexagonal	a=6.10 c=14.47	$[D_{6h}^{4}$-- $P6_3/mmc]$	"	53, 54,55
Al_2Pu	cubic	a=7.831	C15	X-ray powder data.	53,55
~AlPu	cubic			X-ray diffraction data; probably one or more forms of a distorted B2 structure; a range of solid solubility may exist in this region of the phase diagram.	55
$AlPu_3$	tetragonal	a=4.499 or 4.530 c=4.538 or 4.475	L12	Structure partially ordered; a and c axes interchanged by one investigator on basis of intensity data.	55
Al_4Np	orthorhombic	a=4.42 b=6.26 c=13.71	$[D_{2h}^{28}$-- Imma]	Powder and single crystal x-ray data.	56
Al_3Np	cubic	a=4.262	L12	X-ray powder data.	56
Al_2Np	cubic	a=7.785	C15	"	56
AlB_2	hexagonal	a=3.01 c=3.25	C32	Powder and single crystal x-ray data.	57, 58,160
AlB_4				A probable decomposition product of AlB_2; crystallizes in very low symmetry.	160
AlB_{10}	orthorhombic	a=8.84 b=9.02 c=5.67	$[C_{2v}^{12}$-- $Bb2_1m]$	Single crystal x-ray data; pseudotetragonal.	169
AlB_{12}	monoclinic	a=8.523 b=11.00 c=7.393 β=143° 29'	$[C_{2h}^{3}$-- $C2/m]$ or $[C_2^3$-- $C2]$ or $[C_s^3$-- $Cm]$	Single crystal x-ray data; originally reported as AlB_{13}; reported as orthorhombic (169) with a=12.29, b=12.57, c 1014, space group $[D_{2h}^{28}$--Imma].	59,169

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
AlB_{12}	tetragonal	a=10.14 c=14.26	$[D_4^4$ -- $P4_12_12]$ or $[D_4^8$ -- $P4_32_12]$	Single crystal x-ray data; pseudo-cubic.	59,169
Al_3Ti	tetragonal	a=5.436 c=8.596	DO_{22}	X-ray powder data.	60,64
AlTi	tetragonal	a=4.01-3.99 c=4.07-4.08	L10	X-ray powder data, thermal and micrographic analysis; parameters vary with composition; phase exists from 35.5-44.5 w/o Al at 800°C.	60,61
$AlTi_2$	hexagonal	a=5.775 c=4.638 (25 w/o Al)	DO_{19}	X-ray diffraction data; isomorphous with Ti_3Sn; possible evidence for another compound of higher Ti content; superlattice.	62,63, 143,144
Al-Zr				Thermal analysis shows Zr_2Al (~13 w/o Al), Zr_5Al_3 (~15 w/o Al), Zr_3Al_2 (16.46 w/o Al), Zr_4Al_3 (18.15 w/o Al), ZrAl (22.82 w/o Al), and Zr_2Al_3 (30.72 w/o Al) in addition to the compounds listed below.	66
Al_3Zr	tetragonal	a=4.013 c=17.310	DO_{23}	Single crystal x-ray data.	64,66
Al_2Zr	orthorhombic	a=10.42 b=7.22 c=4.98		X-ray powder data.	66
$AlZr_3$	cubic	a=4.372	L12	"	65,66
Al_3Th	hexagonal	a=6.499 c=4.626	$[D_{6h}^4$ -- $P6_3/mmc]$	X-ray powder data.	67,68
Al_2Th	hexagonal	a=4.393 c=4.164	C32	X-ray powder and neutron diffraction data.	67,68
~Al_7Th_4	tetragonal	a=9.86 c=7.81		X-ray powder data; stable only in a narrow temperature range at ~1300°C; powder sample not single-phase.	67
AlTh	orthorhombic	a=11.45 b=4.42 c=4.19	$[D_2^5$ -- $C222_1]$	Powder and single crystal x-ray data; structure tentative.	67

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Al_2Th_3	tetragonal	a=8.13 c=4.22	D^5_{4h} -- P4/mbm	X-ray powder data; stable only above 1100°C.	67,68
$AlTh_2$	tetragonal	a=7.62 c=5.86	C16	X-ray powder data.	67,68
Al_4C_3	rhombohedral	a=8.55 α=22° 28'	$D7_1$	Single crystal x-ray data.	74
$Al_{10}V$	cubic	a=14.586	O^7_h -- Fd3m	Powder and single crystal x-ray data; range of composition varying from $Al_{10}V$ to $Al_{21}V_2$; originally reported as $Al_{11}V$.	70, 71,72
~Al_7V	monoclinic	a=25.4 b=7.59 c=11.0 β=127°	C^3_{2h} -- C2/m	Single crystal x-ray data; space group tentative.	70,73
$Al_{23}V_4$	hexagonal	a=7.6928 c=17.040	D^4_{6h} -- $P6_3/mmc$	Powder and single crystal x-ray data; originally reported as VAl_6.	69
Al_3V	tetragonal	a=5.345 c=8.322	DO_{22}	X-ray powder data.	70
Al_8V_5	cubic	a=9.207	$D8_2$	X-ray powder data; range of composition variation.	70
Al_3Nb	tetragonal	a=5.438 c=8.601	DO_{22}	X-ray powder data.	64
Al_3Ta	tetragonal	a=5.433 c=8.553	DO_{22}	X-ray powder data, thermal and microscopic analysis.	64,197
AlAs	cubic	a=5.63	B3	X-ray powder data, thermal analysis.	135
AlSb	cubic	a=6.1355	B3	X-ray powder data.	75,78, 79

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Al_7Cr	monoclinic	a=20.47 b=7.64 c=25.36 β=155° 10'		Laue and rotation x-ray data; the cell was originally indexed as orthorhombic by (81), with a=19.99, b=12.47, c 34.51 A.	80,81, 156
$Al_{11}Cr_2$	orthorhombic	a=24.8 b=24.7 c=30.2		X-ray powder data, thermal analysis; there is some discussion of the relationship of this structure to the structure of Al_7Cr included in reference (156).	81,155, 156
Al_4Cr				X-ray powder data, thermal analysis.	81
Al_3Cr				"	81
Al_9Cr_4				X-ray powder data, thermal analysis; two phases similar in structure are present in this region, with composition ranges so nearly the same they are represented by the same formula.	81
Al_8Cr_5	rhombohedral	a=7.805 α=109° 7.6'	$D8_{10}$	X-ray powder data; this structure is pseudo-cubic and is closely related to the γ-brass structure.	81, 82,83
$AlCr_2$	tetragonal	a=3.004 c=8.647	C48	X-ray powder data.	82
Al-Mo				Thermal analysis indicates the existence of $MoAl_5$, $MoAl_2$ or 3, Mo_3Al, and possibly another compound between the latter two.	87,88
$Al_{12}Mo$	cubic	a=7.573	$[T_h^5$-- Im3]	X-ray powder data.	86
$AlMo_3$	cubic	a=4.9495	A15	X-ray powder data, metallography.	87
$Al_{12}W$	cubic	a=7.580	$[T_h^5$-- Im3]	X-ray powder data.	86
Al_5W	hexagonal	a=4.9020 c=8.8570	$[C_6^6$-- $P6_3]$	Powder and single crystal x-ray data.	89
Al_4W	monoclinic	a=5.272 b=17.771 c=5.218 β=100° 12'	$[C_s^3$-- Cm]	Single crystal x-ray data.	76

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
Al_4U	ortho-rhombic	a=4.41 b=6.27 c=13.71	C_{2v}^{22} -- I2ma or D_{2h}^{28} -- Imma	Single crystal x-ray data.	90
Al_3U	cubic	a=4.287	L12	X-ray powder data.	91
Al_2U	cubic	a=7.811	C15	"	91
Al_2Se_3	hexag-onal	a=3.89 c=6.30	B4	X-ray powder data; a second modification exists at higher temperatures.	92
Al_5Te				Thermal analysis.	94,95
Al_2Te_3				"	93, 94,95
$\sim Al_{12}Mn$	cubic	a=13.28		X-ray powder data, thermal analysis; metastable phase formed on annealing below 550°C.	98,99
Al_6Mn	ortho-rhombic	a=6.4978 b=7.5518 c=8.8703	D_{2h}^{17} -- Ccmm	Single crystal x-ray data; previously reported as $MnAl_7$, $MnAl_5$, or $MnAl_4$.	96,97, 100
Al_4Mn	hexag-onal	a=28.41 c=12.38		X-ray powder data.	100
Al_3Mn	ortho-rhombic	a=14.82 b=12.63 c=12.46		X-ray powder data; thermal analysis.	100, 101, 134
$Al_{11}Mn_4$	tri-clinic	a=5.092 b=8.862 c=5.047 α=85° 19', β=100° 24' γ=105° 20'	C_i^1 -- P$\bar{1}$	Single crystal x-ray data; pseudo-monoclinic.	77
AlMn	cubic	a≈2.98	B2	X-ray powder data, thermal analysis; wide range of homogeneity from 49-67 w/o Mn.	102, 134
Al_7Fe_2				On the basis of x-ray powder diagrams (110) maintains that this phase is distinct and different from $FeAl_3$; however, there is no question but that the diffraction patterns are very similar.	109, 110, 111

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
Al_3Fe	monoclinic	a=15.489 b=8.0831 c=12.475 β=107° 43'	C_{2h}^3 -- C2/m	Single crystal x-ray data.	105
Al_5Fe_2	orthorhombic	a=7.575 b=6.403 c=4.203	D_{2h}^{17} -- Cmcm	Single crystal x-ray data, thermal and microscopic analysis; previously reported as monoclinic.	97,112, 113, 114
Al_2Fe	rhombohedral	a 6.327 α 87° 24'		X-ray powder data, thermal and microscopic analysis; α reported as 74°09' by (113); (106) reports the existence in this region of an additional high temperature orthorhombic phase which cannot be retained on quenching.	106, 113, 114, 157
AlFe	cubic	a=2.908	B2	X-ray powder data, thermal analysis.	103,104
$AlFe_2$	hexagonal		C14	Unstable phase claimed to be present in a complex Fe-Ni-Cr alloy.	107
$AlFe_3$	cubic	a 5.792	DO_3	X-ray powder data, thermal analysis.	103, 104,108
Al_9Co_2	monoclinic	a=8.5565 b=6.290 c=6.2130 β=94.760°	C_{2h}^5 -- $P2_1/a$	Single crystal x-ray data.	115, 116, 120
$Al_{13}Co_4$				Complicated powder pattern.	116
Al_3Co				Qualitative x-ray study indicates possible existence of this phase.	116
Al_5Co_2	hexagonal	a=7.671 c=7.608	$D8_{11}$	X-ray powder data.	116, 117
AlCo	cubic	a=2.862	B2	"	116, 118
Al_3Ni	orthorhombic	a 6.611 b 7.366 c=4.812	DO_{20}	X-ray powder data.	120, 121, 122,123
Al_3Ni_2	hexagonal	a=4.036 c=4.900	$D5_{13}$	X-ray powder data; powder data from a quenched alloy (126) gives tetragonal with a=2.668, c=3.244 Å with 1 Ni at 000, 0.8 Al and 0.2 Ni randomly at $\frac{1}{3}\frac{1}{3}\frac{1}{3}$.	119, 122, 123, 126

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
AlNi	cubic	a=2.880 (49.4 a/o Ni)	B2	Powder and single crystal x-ray data; thermal analysis.	121,123, 124,125
$AlNi_3$	cubic	a=3.57-3.59	L12	X-ray powder data, thermal analysis; lattice varies with heat treatment given alloy.	123, 124, 125
AlRh	cubic	a=2.99	B2	X-ray analysis.	84,170
Al_3Pd	orthorhombic	a=7.085 b=7.531 c=5.087	$[D_{2h}^{12}$-- Pnnm] or $[C_{2v}^{10}$-- Pnn2]	X-ray powder data, thermal analysis.	127, 129
Al_3Pd_2	hexagonal	a=4.21 c=5.14 (40 a/o Pd)	$D5_{13}$	"	127, 128, 129,130
α-AlPd	monoclinic	a=9.70 b=15.17 c=5.25 β=78.90°		X-ray powder data, thermal analysis; low temperature modification; according to (127) this phase is hexagonal with a 3.958, c 5.614 A.	84, 127, 129
β-AlPd	cubic	a=3.046	B2	X-ray powder data, thermal analysis; high temperature modification (above 900°C).	128, 129, 130
$AlPd_2$	orthorhombic	a=7.776 b=5.415 c=4.057	$[D_{2h}^{16}$-- Pnam]	X-ray powder data; thermal and metallographic analysis.	130, 170
AlOs	cubic	a=3.005	B2	X-ray powder data.	84
AlIr	cubic	a=2.983	B2	"	84
Al_3Pt				Thermal analysis. (133) reports an additional intermediate phase of composition $PtAl_6$, but experimental basis for the report is not specified.	132, 133
Al_2Pt	cubic	a=5.922	C1	X-ray powder data.	131
AlPt	cubic	a=4.865	B20	"	84

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
InLi	cubic	$a=6.80_0$	B32	X-ray powder data, thermal analysis.	145,146
InNa	cubic	a=7.312	B32	X-ray powder data; (148) postulates the existence of two additional compounds in the system, In_3Na and In_2Na, from cooling curves.	147, 148
In_3Cu_7	tetragonal	a=8.99 c=9.16		X-ray powder data, thermal analysis; exists below 630°C; tetragonally distorted cube; related to the γ-brass structures.	150, 158
$\sim In_4Cu_9$	cubic	a=9.250 (29.6 a/o In)	$D8_{1-3}$	High temperature x-ray powder data; thermal analysis; exists above 610°C.	150, 158, 159
$InCu_2$	hexagonal	a=4.277 c=5.249 (35.6 a/o In)	B8	X-ray powder data, thermal analysis; phase extends from 32.4-38.8 a/o In at room temperature; lattice parameters vary with composition.	150, 152, 153
$\sim InCu_4$	cubic	a=3.046 (at 672°C)	A2	X-ray powder data, thermal analysis; exists above 574°C; ideal formula would be $InCu_3$ in accord with theory for 3:2 electron compounds (167).	20, 150, 151, 164,167
In_2Ag	tetragonal	a=6.883 c=5.616	C16	X-ray powder data, thermal analysis.	154, 164
$InAg_2$	cubic	a=9.905	$D8_{1-3}$	X-ray powder data, thermal analysis; an order-disorder transformation occurs at 204°C; the difference between the two modifications cannot be detected with x-rays.	154, 164
$InAg_3$	hexagonal	a=2.954 c=4.804		X-ray powder data, thermal analysis; parameters vary slightly with composition; an order-disorder transformation occurs at 187°C; the lower-temperature phase has the hexagonal DO_{19} structure; in addition, a high temperature cubic disordered phase exists between 660 and 693°C.	154, 164, 167

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS(Å)	STRUCTURE	REMARKS	REFERENCES
In_2Au	cubic	a=6.515	C1	X-ray powder data; thermal and microscopic analysis.	131, 164, 168
InAu	triclinic	a=4.30 b=10.59 c=3.54 α=70.54°, β=90.00° γ=90.17°		X-ray and thermal analysis; pseudo-orthorhombic.	112, 168
In_4Au_9	cubic	a=9.82	$D8_{1-3}$	X-ray powder data; thermal and microscopic analysis; undergoes a transformation around 370°C, probably of order-disorder type.	164, 168
$InAu_3$				On the basis of thermal evidence only, (168) postulates this phase with a very small region of homogeneity; (165) and (170) mention an orthorhombic compound with this formula with the Cu_3Ti type structure, a=5.86, b=5.17, c=4.75 Å.	165, 168, 170
~$InAu_4$	hexagonal	a=2.914 c=4.787 (~12.8 w/o In)	A3	X-ray powder data; thermal and microscopic analysis; homogeneous from 9.8-12.8 w/o In at room temperature; parameters vary slightly with composition.	154, 167, 168
In-Mg				X-ray diffraction data, thermal analysis; disordered f.c.c. phase existing above ~300°C from ~24-54 a/o In; at lower temperatures orders to the L12 structure at ~25 a/o In, to L10 structure around 50 a/o In; orders to an orthorhombic structure at intermediate temperatures and concentrations. (15) postulates the existence of $InMg_{2\ or\ 3}$, which was not found by (187); results of unpublished work are given in (204), reporting 3 intermediate phases with structures and lattice parameters given, but no compositions specified.	15, 166, 187, 204
$InMg_2$				X-ray diffraction data; thermal analysis; exists below 298°C; (166) reports complex structure; (15) reports this compound hexagonal and isomorphous with Mg_2Ga.	15,166

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
~$InMg_3$				X-ray diffraction data; thermal analysis; (15) postulates the existence in this region of orthorhombic In_2Mg_5, isomorphous with Ga_2Mg_5; (156) reports a complex structure.	15,166
InCa				X-ray powder data; structure is noncubic.	149
In-La				(7) draws an analogy between the Ce-In and La-In systems, postulating the existence of $LaIn_3$, La_2In_3, LaIn, La_2In, and La_3In.	7
In-Ce				Thermal analysis indicates the existence of In_3Ce, In_3Ce_2, InCe, $InCe_2$, and $InCe_3$.	7
In_3Ce	cubic	a=4.680	L12	X-ray powder data.	7
In-Pr				X-ray powder, thermal, and micrographic data indicate the existence of In_3Pr, In_3Pr_2, InPr, $InPr_2$, and $InPr_3$.	8
In_3Pr	cubic	a=4.67	L12	X-ray powder data; thermal and micrographic analysis.	8
$InPu_3$	cubic	a=4.703	L12	X-ray powder data; phase is partially ordered.	55
In-Hg				Thermal analysis indicates the existence of 3 compounds: $InHg_5$, InHg, and $In_{11}Hg$.	191
In-Tl	cubic	a=4.7445 (22.73 a/o Tl) a=4.7901 (55.33 a/o Tl)		X-ray diffraction data; thermal analysis; wide range of homogeneity; there was a question as to the existence of a phase boundary between this cubic structure and the tetragonal solid solution region; recent work (201) has confirmed the existence of a narrow two-phase region between the In solid solution and this f.c.c. α-phase.	189, 201, 203

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
$InTi_3$	hexagonal	a=5.89 c=4.76 (~39 w/o In)	DO_{19}	X-ray powder data; (161) reports in addition a cubic phase (possibly the L12 structure) near 40 a/o In, with a=4.22 Å.	143, 161
$InZr_3$	cubic	a=4.461	L12	X-ray powder data, thermal analysis; phase exists from 22.4-28.5 a/o In and possibly to higher In contents which were not investigated; possibly the ordering is incomplete.	137,161
In_3Sn	tetragonal	a=3.470 c=4.391 (24.37 a/o Sn)		X-ray powder data, thermal analysis; region of existence of ~14-27 a/o Sn.	138, 140,172, 173,174
$InSn_4$	hexagonal	a=3.2178 c=2.9990 (18.64 a/o In)	$\left[D^1_{6h}\right]$--P6/mmm	X-ray powder data; thermal and microscopic analysis; region of existence of ~75-88 a/o Sn; monatomic unit cell with random distribution of atomic species.	140, 141, 172, 174, 188
In-Pb	tetragonal	a=4.867 c=4.539 (14.3 a/o Pb) a=4.905 c=4.554 (27 a/o Pb)		X-ray diffraction data, thermal analysis; range of existence of ~14.3-31 a/o Pb; this intermediate phase probably occurs because the difference in crystal structure of Pb and In precludes continuous solid solution.	201, 202, 203
InAs	cubic	a=6.0584	B3	X-ray powder data, thermal analysis.	75,136
InSb	cubic	a=6.47877	B3	"	75,78, 139,183
In_2Bi	hexagonal	a=5.498 c=3.291	C32	X-ray powder data with intensities; thermal and metallographic analysis; from single crystal x-ray data (190) reports a=5.496, c=6.579 Å, space group $\left[D^4_{6h}\right]$--C6/mmc.	142, 176, 190
InBi	tetragonal	a=5.000 c=4.773	B10	X-ray powder data with intensities; thermal and metallographic analysis.	142, 175, 176
In_3U	cubic	a=4.6013	L12	X-ray diffraction data.	185,186

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
In_2Se	ortho-rhombic	a=4.073 b=12.26 c=15.26		X-ray powder data.	177, 178
InSe	rhombo-hedral	a=4.02 c=25.05 (hexagonal cell)		"	177, 178
α-In_2Se_3	hexag-onal	a=3.99 c=19.0		Single crystal x-ray data; high temperature modification; exists above 600-700°C.	171, 178, 184
β-In_2Se_3				Complex powder pattern; low temperature modification; further modifications of In_2Se_3 may exist.	171, 178
In_2Te	ortho-rhombic	a=4.46 b=12.61 c=15.35		X-ray powder data.	177, 178
InTe	tetrag-onal	a=8.437 c=7.139	B37	Powder and single crystal x-ray data; thermal analysis.	178, 179
In_2Te_3	cubic	a=6.146	B3	X-ray powder data, thermal analysis; some metal positions are statistically vacant; from single crystal work (182) reports a=18.40 Å.	178, 180, 181, 182
In_2Te_5	mono-clinic	a=4.38 b=16.11 c=13.37 β=92.05°		X-ray analysis.	177
$InMn_3$	cubic	a=9.435	$D8_{1-3}$	X-ray powder data; thermal and microscopic analysis; from magnetic measurements (193) believes this compound to be Mn_2In, while (194), also on the basis of magnetic measurements, reports Mn_4In.	192, 193, 194
In-Co				Thermal, microscopic, and x-ray analysis by (195) indicates the formation of Co_3In_2, CoIn, and $CoIn_2$.	195, 196

COMPOUND	CRYSTAL CLASS	LATTICE PARAMETERS (Å)	STRUCTURE	REMARKS	REFERENCES
~In_3Ni	cubic	a=9.200	~$D8_{1-3}$	X-ray powder data.	164,198
In_3Ni_2	hexagonal	a=4.396 c=5.302	$D5_{13}$	X-ray powder data; (200) calls this phase $NiIn_2$.	164, 198,200
InNi	cubic	a=3.099	B2	X-ray powder data; high temperature modification; range of homogeneity of ~45-60 a/o In.	164, 198
InNi	hexagonal	a=4.545 c=4.353	B35	X-ray powder data; low temperature modification.	164, 198,199
$InNi_2$	hexagonal	a=4.185 c=5.135	$[D^4_{6h}$-- $P6_3/mmc]$	X-ray powder data; range of homogeneity ~ 33-39 a/o In at lower temperatures.	152, 164, 198,199
$InNi_3$	hexagonal	a=5.331 c=4.251	DO_{19}	X-ray powder data.	164, 198
InRh	cubic	a=3.20	B2	X-ray analysis.	84,170
~In_3Pd	cubic	a=9.44	~$D8_{1-3}$	"	164
In_3Pd_2	hexagonal	a=4.53 c=5.50	$D5_{13}$	"	164
InPd	cubic	a=3.257	B2	"	164
~$InPd_2$	orthorhombic	a=8.24 b=5.61 c=4.22	$[D^{16}_{2h}$-- $Pnam]$	"	164, 170
$InPd_3$	tetragonal	a=4.07 c=3.80	A6	"	164
In_7Pt_3	cubic	a=9.435	$[O^9_h$-- $Im3m]$	X-ray powder data.	128
In_2Pt	cubic	a=6.366	C1	X-ray powder data; stable only at high temperatures.	131
In_3Pt_2	hexagonal	a=4.53 c=5.51	$D5_{13}$	X-ray analysis.	164

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PART III: STRUCTURE DETAILS

A 2: O_h^9--Im3m

A=2: W structure
with 2 W (O_h): $000;\frac{111}{222}$

Reported Compounds: β-$AlCu_3$, β-$AlAg_3$, $InCu_4$

Remarks: Implied in this structure is a random distribution of the atomic species on the lattice sites.

A 3: D_{6h}^4--$P6_3/mmc$

A=2: Mg structure
with 2 Mg (D_{3h}): 2/3,1/3,0; 1/3,2/3,1/2

Reported Compounds: Al_2Ag_3, $InAu_4$

Remarks: See Remarks under A 2 structure.

A 6: D_{4h}^{17}--$F4/mmm$

A=4: In structure
with 4 In (D_{4h}): $000;\frac{11}{22}0;$ ↻

Reported Compounds: $InPd_3$

Remarks: See Remarks under A 2 structure.

A 12: T_d^3--$I\bar{4}3m$

A=58: α-Mn structure
with
2 Mn (T_d): 000+B. C.
8 Mn (C_{3v}): xxx;$\bar{x}\bar{x}x$;↻;+B. C.: x=0.32
24 Mn (C_s): xxz;↻;$\bar{x}\bar{x}z$;↻;$\bar{x}x\bar{z}$;↻;$x\bar{x}\bar{z}$;↻;+B. C.: x=0.36, z=0.04
24 Mn (C_s): the same with x=0.09, z=0.28

[B. C. = add 000 and $\frac{111}{222}$ to all coordinates;↻=permutations]

Reported Compounds: $Al_{12}Mg_{17}$

A 15: O_h^3--Pm3n

A=8: Cr_3Si structure
with
2 Si (T_h): $000;\frac{111}{222}$
6 Cr (D_{2d}): 1/2,0,1/4;↻;1/2,0,3/4;↻

Reported Compounds: $AlMo_3$

B 2: O_h^1--Pm3m

A=2: ordered β-brass or CsCl structure
with 1 Cs (O_h): 000
1 Cl (O_h): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$

Reported Compounds: AlNd, AlMn, AlFe, AlCo, AlNi, AlPd, AlOs, AlIr, AlRh, InPd, InRh, InNi

B 3: T_d^2--F$\bar{4}$3m

A=8: Sphalerite structure, ZnS
with 4 Zn (T_d): 000 + F. C.
4 S (T_d): $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ + F. C.
[F. C.= add 000; $\frac{1}{2}0\frac{1}{2}$; $\frac{1}{2}\frac{1}{2}0$; and $0\frac{1}{2}\frac{1}{2}$ to all coordinates]

Reported Compounds: AlAu, AlAs, AlSb, InAs, InSb, In_2Te_3

Remarks: Some metal sites in In_2Te_3 are statistically vacant.

B 4: C_{6v}^4--P6_3mc

A=4: Wurtzite structure, ZnS
with 2 Zn (C_{3v}): 1/3,2/3,0; 2/3,1/3,1/2
2 S (C_{3v}): 1/3,2/3,z; 2/3,1/3,1/2+z: z≈3/8

Reported Compounds: Al_2Se_3

Remarks: Cell content is 2[$Al_{2/3}Se$]: 2 Se (C_{3v}): 1/3,2/3,0; 2/3,1/3,1/2 and 1 1/3 Al (C_{3v}): 1/3,2/3,z; 2/3,1/3,1/2+z: z=3/8. The selenium atoms lie in the h.c.p. positions; the aluminum atoms occupy 2/3 of the available tetrahedral spaces.

B 8: D_{6h}^4--P6_3/mmc

A=4: α-NiAs structure
with 2 Ni (D_{3d}): 000; $00\frac{1}{2}$
2 As (D_{3h}): 1/3,2/3,1/4; 2/3,1/3,3/4

D_{6h}^4--P6_3/mmc

A=6: β-Ni_2In structure
with 2 Ni (D_{3d}): 000; $00\frac{1}{2}$
2 Ni (D_{3h}): 1/3,2/3,3/4; 2/3,1/3,1/4
2 In (D_{3h}): 1/3,2/3,1/4; 2/3,1/3,3/4

Reported Compounds: $InCu_2$

Remarks: Between the types α and β there exist intermediate arrangements due to deviations in stoichiometry. There exists a close relationship to the C6 structure.

B 10: D_{4h}^{7}--P4/nmm

A 4: LiOH structure
with 2 Li (D_{2d}): 000; $\frac{1}{2}\frac{1}{2}0$
2 OH (C_{4v}): $0\frac{1}{2}z$; $\frac{1}{2}0\bar{z}$: z 0.20

Reported Compounds: InBi with z=0.393

B 20: T^{4}--$P2_13$

A=8: FeSi structure
with 4 Fe (C_3): xxx; $\frac{1}{2}+x,\frac{1}{2}-x,\bar{x}$; ②: x 0.137
4 Si (C_3): the same with x -0.158

Reported Compounds: AlPt with x_{Pt} 0.152, x_{Al} -0.155

B 32: O_h^7--Fd3m

A=16: NaTl structure
with 8 Na (T_d): 000; $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ + F. C.
8 Tl (T_d): 1/2,1/2,1/2; 3/4,3/4,3/4 + F. C.

Reported Compounds: AlLi, InLi, InNa

B 35: D_{6h}^{1}--P6/mmm

A=6: CoSn structure
with 1 Sn (D_{6h}): 000
2 Sn (D_{3h}): 1/3,2/3,1/2; 2/3,1/3,1/2
3 Co (D_{2h}): $\frac{1}{2}00$; $0\frac{1}{2}0$; $\frac{1}{2}\frac{1}{2}0$

Reported Compounds: InNi

B 37: D_{4h}^{18}--I4/mcm

A=16: TlSe structure
with 4 Tl (D_4): 0,0,1/4; 0,0,3/4 + B. C.
4 Tl (D_{2d}): 1/2,0,1/4; 1/2,0,3/4 + B. C.
8 Se (C_{2v}): $\pm(x,\frac{1}{2}+x,0;\ \frac{1}{2}+x,\bar{x},0)$ + B. C.: x=0.179

Reported Compounds: InTe with x=0.18$_0$

C 1: O_h^5--Fm3m

A=12: fluorite structure, CaF_2
with 4 Ca (O_h): 000 + F. C.
8 F (T_d): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ + F. C.

Reported Compounds: θ'-Al_2Cu, Al_2Au, Al_2Pt, In_2Au, In_2Pt

Remarks: The θ'-$CuAl_2$ structure is distorted.

C 14: D_{6h}^4--$P6_3/mmc$

A=12: $MgZn_2$ structure--Laves phase
with 4 Mg (C_{3v}): $\pm(1/3,2/3,z;\ 1/3,2/3,1/2-z)$: z=0.062
2 Zn (D_{3d}): $000;00\frac{1}{2}$
6 Zn (C_{2v}): $\pm(x,2x,\frac{1}{4};\ 2\bar{x},\bar{x},\frac{1}{4};\ x,\bar{x},\frac{1}{4})$: x=-0.170

Reported Compounds: $AlFe_2$

C 15: O_h^7--$Fd3m$

A=24: $MgCu_2$ structure--Laves phase
with 8 Mg (T_d): $000;\frac{111}{444}$+F. C.
16 Cu (D_{3d}): 5/8,5/8,5/8; 7/8,7/8,5/8; 7/8,5/8,7/8; 5/8,7/8,7/8+F. C.

Reported Compounds: Al_2Ca, Al_2La, Al_2Ce, Al_2Pu, Al_2Np, Al_2U

C 16: D_{4h}^{18}--$I4/mcm$

A=12: $CuAl_2$ structure
with 4 Cu (D_4): $\pm(00\frac{1}{4})$ + B. C.
8 Al (C_{2v}^4): $\pm(x,\frac{1}{2}+x,0;\ \frac{1}{2}+x,\bar{x},0)$ + B. C.: x=0.158

Reported Compounds: Θ-Al_2Cu with x=0.160, $AlTh_2$ with x=0.162, In_2Ag with x=0.158

C 32: D_{6h}^1--$P6/mmm$

A=3: AlB_2 structure
with 1 Al (D_{6h}): 000
2 B (D_{3h}): 1/3,2/3,1/2; 2/3,1/3,1/2

Reported Compounds: AlB_2, Al_2Th, In_2Bi

Remarks: For In_2Bi (176) reports 2 In and 1 Bi statistically distributed in (D_{6h}): 000 and (D_{3h}): $\pm(1/3,2/3,1/2)$; (190) reports space group D_{6h}^4--$P6/mmc$, atomic positions 2 Bi in (D_{3h}): $\pm(1/3,2/3,1/4)$, 2 In in (D_{3d}): $000;00\frac{1}{2}$, and 2 In in (D_{3h}): $\pm(1/3,2/3,3/4)$.

C 48: D_{4h}^{17}--$I4/mmm$

A=6: Cr_2Al structure
with 2 Al (D_{4h}): 000+B. C.
4 Cr (C_{4v}): $00z;00\bar{z}$+B. C.: z=0.319

Reported Compounds: $AlCr_2$

D O_3: O_h^5--Fm3m

A=16: $BiLi_3$ structure
with 4 Bi (O_h): 000 + F. C.
4 Li (O_h): $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ + F. C.
8 Li (T_d): $\pm(\frac{1}{4}\frac{1}{4}\frac{1}{4})$ + F. C.

Reported Compounds: β_1-$AlCu_3$, $AlFe_3$

D O_{19}: D_{6h}^4--$P6_3/mmc$

A=8: Ni_3Sn structure
with 2 Sn (D_{3h}): $\pm(1/3,2/3,1/4)$
6 Ni (C_{2v}): $x,2x,1/4$; $2\bar{x},\bar{x},1/4$; $x,\bar{x},1/4$; $\bar{x},2\bar{x},3/4$; $2x,x,3/4$; $\bar{x},x,3/4$: $x=5/6$

Reported Compounds: α-$AlCe_3$ with x=0.829, $AlTi_2$, $InTi_3$, $InNi_3$ with x=0.84

D O_{20}: D_{2h}^{16}--Pnma

A=16: NiAl structure
with 4 Ni (C_s): $\pm(x\frac{1}{4}z;\ \frac{1}{2}+x,\frac{1}{4},\frac{1}{2}-z)$: x=-0.131, z=-0.055
4 Al (C_s): the same with x=0.011, z=0.415
8 Al (C_1): $\pm(xyz;\ \frac{1}{2}+x,\frac{1}{2}-y,\frac{1}{2}-z;\ x,\frac{1}{2}-y,z;\ \frac{1}{2}+x,y,\frac{1}{2}-z)$: x=0.174, y=0.053, z=0.856

Reported Compounds: Al_3Ni

D O_{22}: D_{4h}^{17}--I4/mmm

A=8: $TiAl_3$ structure
with 2 Ti (D_{4h}): 000 + B. C.
2 Al (D_{4h}): $00\frac{1}{2}$ + B. C.
4 Al (D_{2d}): $0\frac{1}{2}\frac{1}{4}$; $\frac{1}{2}0\frac{1}{4}$ + B. C.

Reported Compounds: Al_3Ti, Al_3V, Al_3Nb, Al_3Ta

D O_{23}: D_{4h}^{17}--I4/mmm

A=16: $ZrAl_3$ structure
with 4 Zr (C_{4v}): $\pm(00z)$ + B. C.: z=0.122
4 Al (D_{2h}): $0\frac{1}{2}0$; $\frac{1}{2}00$ + B. C.
4 Al (D_{2d}): $0\frac{1}{2}\frac{1}{4}$; $\frac{1}{2}0\frac{1}{4}$ + B. C.
4 Al (C_{4v}): $\pm(00z)$ + B. C.: z=0.361

Reported Compounds: Al_3Zr

D 1_3: D_{4h}^{17}--I4/mmm

A=10: $BaAl_4$ structure
with 2 Ba (D_{4h}): 000+ B. C.
4 Al (C_{4v}): ±(00z) +B. C.: z=0.380
4 Al (D_{2d}): $0\frac{1}{2}\frac{1}{4}; \frac{1}{2}0\frac{1}{4}$ +B. C.

Reported Compounds: Al_4Ca, Al_4Sr, Al_4Ba, Al_4La, Al_4Ce

D 5_{13}: D_{3d}^{3}--C$\bar{3}$m

A=5: Ni_2Al_3 structure
with 1 Al (D_{3d}): 000
2 Al (C_{3v}): 1/3,2/3,z; 2/3,1/3,$\bar{z}$: z=0.352
2 Ni (C_{3v}): the same with z=0.149

Reported Compounds: Al_3Ni_2, Al_3Pd_2, In_3Ni_2 with z_{Ni}=0.135, z_{In}=0.641, In_3Pd_2 with z_{Pd}=0.138, z_{In}=0.625, In_3Pt_2

D 7_1: D_{3d}^{5}--R$\bar{3}$m

A=7: Al_4C_3 structure
with 1 C (D_{3d}): 000
2 C (C_{3v}): ±(xxx): x=0.217
2 Al (C_{3v}): the same with x=0.293
2 Al (C_{3v}): the same with x=0.128

Reported Compounds: Al_4C_3

D 8_{1-3}: O_h^9--Im3m; T_d^3--I$\bar{4}$3m; and T_d^1--P$\bar{4}$3m

A=52: γ-brass structures. The basic structure consists of a cubic unit cell whose edge is three times the edge of a simple body-centered cubic cell. From this large cell of 54 atomic sites are abstracted 2 atomic sites with small attendant shifts in parameters of some of the 52 occupied sites. The space group depends upon the formula of the compound and the atomic species occupying the various atomic sites. γ-brass structures usually exhibit extensive composition variation.

Reported Compounds: η-AlCu, Al_3Cu_4, Al_2Cu_3, Al_4Cu_9, Al_8V_5, In_4Cu_9, $InAg_2$, In_4Au_9, $InMn_3$, ~In_3Ni, ~In_3Pd

D 8_{10}: C_{3v}^5--R3m

A=26: Cr_5Al_8 structure
with 1 Cr (C_{3v}): xxx: x=0.097
3 Cr (C_s): xxz; ② : x=-0.103, z=0.106
3 Cr (C_s): the same with x=0.170, z=-0.172
3 Cr (C_s): the same with x=0.003, z=0.352
1 Al (C_{3v}): xxx: x=-0.164
3 Al (C_s): xxz; ② : x=0.006, z=-0.352
3 Al (C_s): the same with x=0.291, z=0.058
3 Al (C_s): the same with x=-0.322, z=0.044
6 Al (C_1): xyz; ② ;xzy; ② : x=0.330, y=-0.297, z=-0.042

Reported Compounds: Al_8Cr_5

D 8_{11}: D_{6h}^4--$P6_3/mmc$

A=28: Co_2Al_5 structure
with 2 Co (D_{3h}): 2/3,1/3,1/4; 1/3,2/3,3/4
6 Co (C_{3v}): $\pm(x,2x,\frac{1}{4};\ 2\bar{x},\bar{x},\frac{1}{4};\ x\bar{x}\frac{1}{4})$: x=0.128
2 Al (D_{3d}^{2v}): $000;00\frac{1}{2}$
6 Al (C_{2v}): $\pm(x,2x,\frac{1}{4};\ 2\bar{x},\bar{x},\frac{1}{4};\ x\bar{x}\frac{1}{4})$: x=0.467
12 Al (C_s): $\pm(2x,x,z;\ \bar{x},2\bar{x},z;\ \bar{x}xz;\ 2\bar{x},\bar{x},\frac{1}{2}+z;\ x,2x,\frac{1}{2}+z;$
$x,\bar{x},\frac{1}{2}+z)$: x=0.196, z=0.061

Reported Compounds: Al_5Co_2

L 10: D_{4h}^1--C4/mmm

A=4: CuAu structure
with 2 Cu (D_{4h}): 000 + B. C.
2 Au (D_{4h}): $\frac{1}{2}0\frac{1}{2}$ + B. C.

Reported Compounds: AlTi

L 12: O_h^1--Pm3m

A=4: Cu_3Au structure
with 1 Au (O_h): 000
3 Cu (D_{4h}): $\frac{1}{2}0\frac{1}{2};0\frac{1}{2}\frac{1}{2};\frac{1}{2}\frac{1}{2}0$

Reported Compounds: β-$AlCe_3$, $AlPu_3$, Al_3Np, $AlZr_3$, Al_3U, $AlNi_3$, In_3Pr, In_3Ce, $InPu_3$, $InZr_3$, In_3U

-- C_i^1--$P\bar{1}$

A=15: $Al_{11}Mn_4$ structure
with 2 Mn (C_1): ±(xyz): x=0.3926, y=0.1334, z=0.3390
2 Mn (C_1): the same with x=0.8590, y=0.4022, z=0.7099
1 Al (C_i): 000
2 Al (C_1): ±(xyz): x 0.5339, y=0.1226, z=0.8462
2 Al (C_1): the same with x=0.8911, y=0.1264, z=0.4906
2 Al (C_1): the same with x=0.3420, y=0.3716, z=0.5778
2 Al (C_1): the same with x=0.7242, y=0.3714, z=0.1960
2 Al (C_1): the same with x=0.1869, y=0.3200, z=0.0574

-- C_{2h}^3--C2/m

A=100: Al_3Fe structure
with 4 Fe (C_s): ±(x0z)+C. C.: x=0.086, z=0.383
4 Fe (C_s): the same with x=0.401, z 0.624
4 Fe (C_s): the same with x=0.090, z 0.989
4 Fe (C_s): the same with x=0.400, z=0.985
8 Fe (C_1): ±(xyz;x$\bar{y}$z)+C. C.: x=0.318, y=0.285, z=0.277
4 Al (C_s): ±(x0z)+C. C.: x=0.064, z=0.173
4x0.7 Al (C_s): the same with x=0.322, z=0.277
4 Al (C_s): the same with x=0.235, z=0.539
4 Al (C_s): the same with x=0.081, z=0.582
4 Al (C_s): the same with x=0.231, z=0.972
4 Al (C_s): the same with x=0.480, z=0.827
2 Al (C_{2h}): $\frac{1}{2}0\frac{1}{2};0\frac{11}{22}$
4 Al (C_s): ±(x0z)+C. C.: x=0.086, z=0.781
4 Al (C_s): the same with x=0.310, z=0.769
8 Al (C_1): ±(xyz;x$\bar{y}$z)+C. C.: x=0.188, y=0.216, z=0.111
8 Al (C_1): the same with x=0.373, y=0.211, z=0.107
8 Al (C_1): the same with x=0.176, y=0.216, z=0.334
8 Al (C_1): the same with x=0.495, y=0.283, z=0.329
8 Al (C_1): the same with x=0.366, y=0.223, z=0.479
4 Al (C_2): 0y0;0$\bar{y}$0+C. C.: y=0.244
[C. C.= add 000 and $\frac{11}{22}0$ to all coordinates.]

-- C_s^3--Cm

A=30: Al_4W structure
with 2 W (C_s): x0z+C. C.: x=0, z=0
4 W (C_1): xyz;x$\bar{y}$z+C. C.: x=0.335, y=0.137, z=0.331
2 Al (C_s): x0z+C. C.: x=0.125, z=0.491
2 Al (C_s): the same with x=0.494, z=0.129
4 Al (C_1): xyz;x$\bar{y}$z+C. C.: x 0.674, y=0.076, z=0.687
4 Al (C_1): the same with x=0.824, y=0.118, z=0.213
4 Al (C_1): the same with x=0.181, y=0.129, z=0.809
4 Al (C_1): the same with x=0.682, y=0.232, z=0.583
4 Al (C_1): the same with x=0.005, y=0.245, z=0.090

-- C_{2h}^5 --$P2_1/a$

A=22: Al_9Co_2 structure
with 4 Co (C_1): xyz; $\bar{x}\bar{y}\bar{z}$; $\frac{1}{2}-x,\frac{1}{2}+y,\bar{z}$; $\frac{1}{2}+x,\frac{1}{2}-y,z$: x=0.3335, y=0.6149, z=0.2646
4 Al (C_1): the same with x=0.2682, y=0.9619, z=0.4044
4 Al (C_1): the same with x=0.2309, y=0.2899, z=0.0889
4 Al (C_1): the same with x=-0.0014, y=0.1931, z=0.3891
4 Al (C_1): the same with x=0.0417, y=0.6148, z=0.2159
2 Al (C_i): 000; $\frac{1}{2}\frac{1}{2}0$

-- C_6^6--$P6_3$

A=12: Al_5W structure
with 2 W (C_3): 1/3,2/3,z; 2/3,1/3,1/2+z: $z=\frac{1}{2}$
2 Al (C_3): the same with z=0
2 Al (C_3): 00z; 0,0,$\frac{1}{2}$+z: z=0
6 Al (C_1): xyz; $\bar{y}$,x-y,z; y-x,$\bar{x}$,z; $\bar{x}$,$\bar{y}$,$\frac{1}{2}$+z; y,y-x,$\frac{1}{2}$+z; x-y,x,$\frac{1}{2}$+z: x=y=1/3, z=1/4

-- D_{6h}^4--$P6_3/mmc$

A=24: Al_3Pu structure
with 2 Pu (D_{3h}): $\pm(00\frac{1}{4})$
4 Pu (C_{3v}): $\pm$(1/3,2/3,z; 1/3,2/3,1/2-z): z=0.0892
6 Al (C_{2v}): $\pm(x,2x,\frac{1}{4}; 2\bar{x},\bar{x},\frac{1}{4}; x,\bar{x},\frac{1}{4})$: x=0.5160
12 Al (C_s): $\pm$(x,2x,z; 2$\bar{x}$,$\bar{x}$,z; x$\bar{x}$z; $\bar{x}$,2$\bar{x}$,$\frac{1}{2}$+z; 2x,x,$\frac{1}{2}$+z; $\bar{x}$,x,$\frac{1}{2}$+z): x=0.8337, z=0.0815

-- D_{6h}^4--$P6_3/mmc$

A=6: $InNi_2$ structure
with 2 In (D_{3h}): $\pm$(1/3,2/3,1/4)
2 Ni (D_{3h}): 000; $00\frac{1}{2}$
2 Ni (D_{3h}): $\pm$(1/3,2/3,3/4)

-- D_{6h}^4--$P6_3/mmc$

A=54: $Al_{23}V_4$ structure
with 2 V (D_{3d}): 000; $00\frac{1}{2}$
6 V (C_{2v}): $\pm(x,2x,\frac{1}{4}; 2\bar{x},\bar{x},\frac{1}{4}; x\bar{x}\frac{1}{4})$: x=0.781
12 Al (C_s): $\pm$(x,2x,z; 2$\bar{x}$,$\bar{x}$,z; x$\bar{x}$z; $\bar{x}$,2$\bar{x}$,$\frac{1}{2}$+z; 2x,x,$\frac{1}{2}$+z; $\bar{x}$,x,$\frac{1}{2}$+z): x=0.213, z=0.029
12 Al (C_s): the same with x=0.124, z=0.618
12 Al (C_s): the same with x=0.455, z=0.166
6 Al (C_{2v}): $\pm(x,2x,\frac{1}{4}; 2\bar{x},\bar{x},\frac{1}{4}; x\bar{x}\frac{1}{4})$: x=0.126
4 Al (C_{3v}): $\pm$(1/3,2/3,z; 2/3,1/3,1/2+z): z=0.167*

*The z-parameter for the 4 al (C_{3v}) position is given incorrectly as 0.167 in the literature (see reference No. 69).

-- D_{6h}^4--$P6_3/mmc$

A=8: Al_3Th structure
with 2 Th (D_{3h}): $\pm(2/3,1/3,1/4)$
6 Al (C_{2v}): $\pm(x,2x,\frac{1}{4};\ 2\bar{x},\bar{x},\frac{1}{4};\ x\bar{x}\frac{1}{4})$: x=0.143

-- D_2^5--$C222_1$

A=8: AlTh structure
with 4 Th (C_2): $xx0;\bar{x}0\frac{1}{2}$ +C. C.: x=0.147
4 Al (C_2): the same with x=0.443

-- D_{4h}^5--$P4/mbm$

A=10: Al_2Th_3 structure
with 2 Th (C_{4h}): $000;\frac{1}{2}\frac{1}{2}0$
4 Th (C_{2v}): $\pm(x,\frac{1}{2}+x,\frac{1}{2};\ \frac{1}{2}+x,\bar{x},\frac{1}{2})$: x=0.674
4 Al (C_{2v}): $\pm(y,\frac{1}{2}+y,0;\ \frac{1}{2}+y,\bar{y},0)$: y=0.116

-- D_{2h}^{16}--Pnam

A=12: "corrected" Co_2Si structure
with 4 Co (C_s): $\pm(xy\frac{1}{4};\ \frac{1}{2}-x,\frac{1}{2}+y,3/4)$: x=0.038, y=0.218
4 Co (C_s): the same with x=0.174, y=0.562
4 Si (C_s): the same with x=0.702, y=0.611

Reported Compounds: $InPd_2$, $AlPd_2$

-- D_{2h}^{17}--Cmcm

A≈13: Al_5Fe_2 structure
with 4 Fe (C_{2v}): $\pm(0y\frac{1}{4})$ + C. C.: y=0.332
8 Al (C_s): $\pm(xy\frac{1}{4};\bar{x}y\frac{1}{4})$ + C. C.: x=0.18, y=0.65
0.7 Al (C_{2h}): statistically at $000;00\frac{1}{2}$ +C. C.

Remarks: Evidently a high percentage of the sites in the four-fold position are unoccupied, and the symmetry would indicate that the vacancies are random.

-- D_{2h}^{17}--Ccmm

A=28: Al_5Mn structure
with 4 Mn (C_{2v}): $\pm(x0\frac{1}{4})$ + C. C.: x=0.457
8 Al (C_2): $\pm(0y0;0y\frac{1}{2})$ + C. C.: y=0.327
8 Al (C_s): $\pm(x0z;\ x,0,\frac{1}{2}-z)$ + C. C.: x=0.140, z=0.100
8 Al (C_s): $\pm(xy\frac{1}{4};\bar{x}y\frac{1}{4})$ + C. C.: x=0.290, y=0.320

-- D_{2h}^{28}--Imma

A=20: Al_4U structure
with 4 U (C_{2v}): $\pm(0\frac{1}{4}z)$ + B. C.: z=0.111
4 Al (C_{2v}): the same with z=-0.111
4 Al (C_{2h}): $00\frac{1}{2};0\frac{11}{22}$ + B. C.
8 Al (C_s): $\pm(0yz;\ 0,\frac{1}{2}+y,\bar{z})$ + B. C.: y=-0.033, z=0.314

Reported Compounds: Al_4Pu, Al_4Np, Al_4U

Remarks: Space group for Al_4U may also be [C_{2v}^{22}--I2ma].

-- O_h^7--Fd3m

A=176-184: $Al_{10}V$ structure
with 16 V (D_{3d}): $000;0\frac{11}{44};②$ + F. C.
96 Al (C_s): $\pm(xxz;②;\ x,\frac{1}{4}-x,\frac{1}{4}-z;②;\ \frac{1}{4}-x,\frac{1}{4}-x,z;②)$ + F. C.: x=0.0654, z=0.3009
48 Al (C_{2v}): $\pm(x,1/8,1/8;②;1/4-x,1/8,1/8;②)$ + F. C.: x=0.1407
16 Al (D_{3d}): $\frac{111}{222};\frac{111}{244};②$ + F. C.
8 Al (T_d): $\pm(3/8,3/8,3/8)$ + F. C.

Remarks: The eight-fold set may or may not be occupied by Al atoms. Occupancy of these positions is evidently not necessary for the stability of the structure.

-- O_h^9--Im3m

A=40: In_7Pt_3 structure
with 12 Pt (C_{4v}): $\pm(x00);②$: $x=0.34_2$
12 In (D_{4v}): $\pm(\frac{1}{4}0\frac{1}{2};\frac{1}{2}\frac{1}{4}0;0\frac{1}{2}\frac{1}{4})$
16 In (C_{3v}^{2d}): $\pm(xxx;\bar{x}\bar{x}\bar{x};②)$: $x=0.15_8$

-- T_h^5--Im3

A=26: $Al_{12}W$ structure
with 2 W (T_h): $000;\frac{111}{222}$
24 Al (C_s): $1(0yz;z0y;yz0;0y\bar{z};\bar{z}0y;y\bar{z}0)$ + B. C.: y=0.184, z=0.309

Reported Compounds: $Al_{12}W$, $Al_{12}Mo$